

# Hole-pair symmetry and excitations in the strong-coupling extended $t - J_z$ model

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We analytically calculate the ground state pairing symmetry and excitation spectra of two holes doped into the half-filled  $t - t' - t'' - J_z$  model in the strong-coupling limit ( $J_z \gg |t|, |t'|, |t''|$ ). For the  $t' - t'' - J_z$  model, there are regions of  $d$ -wave,  $s$ -wave, and  $p$ -wave symmetry. We find that the  $t - J_z$  model maps in lowest order onto the  $t' - t'' - J_z$  model on the boundary between  $d$  and  $p$  symmetry, with a flat lower branch of the pair excitation spectrum. In higher order  $d$ -wave symmetry is selected; however, we predict that the addition of the appropriate  $t'$  and/or  $t''$  should drive the hole-pair symmetry to  $p$ -wave. We perturbatively construct an extended quasi-pair for the  $t - J_z$  model. We compare with analytic calculations for a  $2 \times 2$  plaquette and numerical work, and discuss implications for the experimentally relevant parameter regime.

Although the issue has not been completely resolved, a variety of experiments has indicated that the pair symmetry in the hole-doped cuprate superconductors is either pure  $d_{x^2-y^2}$  or has a strong  $d_{x^2-y^2}$  component [1,2]. Theoretical and numerical studies of the two-dimensional Hubbard,  $t - J$ , and related models believed relevant to the high- $T_c$  compounds have also suggested  $d_{x^2-y^2}$  pairing [3–6], and Hubbard and  $t - J$  models on  $2 \times 2$  plaquettes have recently provided an intuitive picture of how such a pair symmetry might arise [7,8]. However, there are few rigorous theoretical results in this general area.

Recent experimental work has indicated that a pseudogap with the same symmetry as the superconducting gap can persist above  $T_c$  in underdoped cuprate superconductors [1,9–11]. This, along with the short high- $T_c$  coherence length [3], is generally consistent with a strong-coupling picture, where pairs can preform at  $T > T_c$  [12]. Numerical work has in addition suggested that the  $t - J$  and  $t - J_z$  models have many similar properties [3,13,14], and that the  $t - J_z$  model may hence provide a suitable starting point for understanding  $t - J$  behavior [15]. In this Letter, we consider two holes doped into the half-filled  $t - t' - t'' - J_z$  model in the strong coupling limit ( $J_z \gg |t|, |t'|, |t''|$ ). We calculate the symmetry of the hole pair in the ground state as well as the pair excitation spectrum. We consider first the  $t' - J_z$  model, and show how singlet pairs can be constructed from our solutions. We next discuss the  $t' - t'' - J_z$  model, and then the  $t - J_z$  and  $t - t' - t'' - J_z$  models. For the  $t - J_z$  model, we perturbatively construct an extended quasi-pair. As a step towards exploring the range of validity of our approach, we compare with results for a  $2 \times 2$  plaquette and numerical studies. Lastly, we discuss implications of our results for the physically relevant parameter regime, including the question of the sufficiency of the  $t - t' - t'' - J$  model for capturing high- $T_c$  behavior.

Specifically, we consider the Hamiltonian

$$H = H_0 + H_1 + H_2 + H_3, \quad (1)$$

where

$$H_0 = J_z \sum_{x,y} \{ (S_{x,y}^z S_{x+1,y}^z + S_{x,y}^z S_{x,y+1}^z) - \frac{1}{4} (n_{x,y} n_{x+1,y} + n_{x,y} n_{x,y+1}) \}, \quad (2)$$

$$H_1 = (-t) \sum_{x,y,\sigma} \{ (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x+1,y,\sigma} + H.c.) + (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x,y+1,\sigma} + H.c.) \}, \quad (3)$$

$$H_2 = (-t') \sum_{x,y,\sigma} \{ (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x+1,y+1,\sigma} + H.c.) + (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x+1,y-1,\sigma} + H.c.) \}, \quad (4)$$

and

$$H_3 = (-t'') \sum_{x,y,\sigma} \{ (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x+2,y,\sigma} + H.c.) + (\tilde{c}_{x,y,\sigma}^\dagger \tilde{c}_{x,y+2,\sigma} + H.c.) \}. \quad (5)$$

Here,  $x$  and  $y$  denote the coordinates of an  $L \times L$  lattice with periodic boundary conditions and even  $L$ , and  $\sigma = \pm 1$  ( $\uparrow, \downarrow$ ) refers to electron spin.  $\tilde{c}_{x,y,\sigma} = c_{x,y,\sigma} (1 - n_{x,y,-\sigma})$ , enforcing the condition of no double occupancy.  $S_{x,y}^z = 1/2 (n_{x,y,\uparrow} - n_{x,y,\downarrow})$  and  $n_{x,y} = n_{x,y,\uparrow} + n_{x,y,\downarrow}$ . We do not explicitly consider here the spin-flip part of the magnetic interaction

$$H_\perp = \left( \frac{J_\perp}{2} \right) \sum_{x,y} \{ (S_{x,y}^+ S_{x+1,y}^- + S_{x,y}^- S_{x,y+1}^+) + H.c. \}, \quad (6)$$

where  $S_{x,y}^+ = c_{x,y,\uparrow}^\dagger c_{x,y,\downarrow}$  and  $S_{x,y}^- = c_{x,y,\downarrow}^\dagger c_{x,y,\uparrow}$ . (The full  $t - t' - t'' - J$  model is recovered when  $J_\perp = J_z$ .)

At half filling each site is occupied by exactly one electron, and the doubly degenerate ground state of  $H_0$  is then that of a Néel antiferromagnet. We choose  $|\Phi_a\rangle$  to denote the state with electron spins  $\sigma(x,y) = (-1)^{x+y}$  and  $|\Phi_b\rangle$  to denote the state with  $\sigma(x,y) = (-1)^{x+y+1}$ . We define the operator  $a_{x,y} = c_{x,y,\sigma(x,y)}$  with  $\sigma(x,y) = (-1)^{x+y}$ , and the operator  $b_{x,y} = c_{x,y,\sigma(x,y)}$  with  $\sigma(x,y) = (-1)^{x+y+1}$ . Although our calculations and results are independent of the ordering convention chosen, we will denote for specificity

$$|\Phi_a\rangle = (a_{L,L}^\dagger \dots a_{1,L}^\dagger) \dots (a_{L,2}^\dagger \dots a_{1,2}^\dagger) (a_{L,1}^\dagger \dots a_{1,1}^\dagger) |0\rangle, \quad (7)$$

with an analogous definition for  $|\Phi_b\rangle$ .

We now dope the half-filled state  $|\Phi_a\rangle$  with two holes and consider the strong-coupling limit ( $J_z \gg |t|, |t'|, |t''|$ ). In this limit, there will be an energy cost of order  $J_z$  if the two holes are *not* nearest neighbors (n.n.). Hence, to zeroth order, the (highly degenerate) two-hole ground state is spanned by the set of all n.n. hole pairs. We denote the state with a horizontal n.n. hole pair at sites  $(x, y)$  and  $(x+1, y)$  as

$$|h_{x,y}\rangle = a_{x+1,y}a_{x,y}|\Phi_a\rangle, \quad (8)$$

and the state with a vertical n.n. hole pair at sites  $(x, y)$  and  $(x, y+1)$  as

$$|v_{x,y}\rangle = a_{x,y+1}a_{x,y}|\Phi_a\rangle. \quad (9)$$

The  $|h_{x,y}\rangle$ 's and  $|v_{x,y}\rangle$ 's provide a complete, orthonormal basis for the two-hole ground state of  $H_0$ .

It costs an energy of order  $J_z$  if one of the n.n. holes hops to a n.n. site through the hybridization matrix element  $t$ . However, there is no energy cost for hops corresponding to  $t'$  or  $t''$ , as long as the two holes remain nearest neighbors after the hop. Thus, to lowest order in  $1/J_z$ , it is only necessary to diagonalize the Hamiltonian  $H_2 + H_3$  in the subspace spanned by the  $|h_{x,y}\rangle$ 's and  $|v_{x,y}\rangle$ 's; i.e., it is only necessary to consider the  $t' - t'' - J_z$  model. We note that in this limit the  $t' - t'' - J_z$  model becomes isomorphic to the strong-coupling limit of the antiferromagnetic van Hove model of [16].

We consider first the  $t' - J_z$  model, involving only the  $H_2$  (diagonal) hopping term. Defining

$$|h_{k_x,k_y}\rangle = \frac{1}{L} \sum_{x,y} e^{-\frac{2\pi i k_x x}{L}} e^{-\frac{2\pi i k_y y}{L}} |h_{x,y}\rangle \quad (10)$$

and

$$|v_{k_x,k_y}\rangle = \frac{1}{L} \sum_{x,y} e^{-\frac{2\pi i k_x x}{L}} e^{-\frac{2\pi i k_y y}{L}} |v_{x,y}\rangle, \quad (11)$$

with  $k_x, k_y = 0, 1, \dots, L-1$ , we obtain the lowest order wave functions

$$|\psi_{k_x,k_y}^\pm\rangle = \frac{1}{\sqrt{2}} \left\{ e^{-\frac{\pi i k_x x}{L}} |h_{k_x,k_y}\rangle \pm \text{sgn}(t') e^{-\frac{\pi i k_y y}{L}} |v_{k_x,k_y}\rangle \right\} \quad (12)$$

with energies

$$\epsilon_{k_x,k_y}^\pm = \pm 4 |t'| \sin\left(\frac{\pi k_x}{L}\right) \sin\left(\frac{\pi k_y}{L}\right). \quad (13)$$

Since  $0 \leq \sin(\pi k_x/L), \sin(\pi k_y/L) \leq 1$ , the minus sign gives the branch of lower energy. The lowest energy state  $|\psi_0^{(a)}\rangle$ , with energy  $-4|t'|$ , occurs when  $k_x = L/2$  and  $k_y = L/2$  (i.e.,  $(\pi, \pi)$ ). Rewriting in terms of the  $a_{x,y}$ 's and neglecting overall phase factors, one obtains

$$|\psi_0^{(a)}\rangle = \frac{1}{L\sqrt{2}} \sum_{x,y} (-1)^{x+y} \{ a_{x+1,y} a_{x,y} - \text{sgn}(t') a_{x,y+1} a_{x,y} \} |\Phi_a\rangle. \quad (14)$$

When  $t' > 0$  ( $\text{sgn}(t') = 1$ ), the sum over hole pair operators in Eq. 14 changes sign upon a 90 degree rotation around a lattice point, giving the pair  $d$ -wave symmetry (specifically,  $d_{x^2-y^2}$  [2,6]). When  $t' < 0$ , there are no such sign changes, giving  $s$ -wave symmetry (specifically, extended- $s$  [2,6]).

If one adds to Eq. 14 the appropriately-phased pair operator for two holes doped into the ground state  $|\Phi_b\rangle$ , one obtains for  $t' > 0$  the usual (unnormalized) n.n. singlet  $d_{x^2-y^2}$  pair operator

$$\frac{1}{L} \sum_{x,y} \left\{ (c_{x,y,\uparrow} c_{x+1,y,\downarrow} - c_{x,y,\downarrow} c_{x+1,y,\uparrow}) - (c_{x,y,\uparrow} c_{x,y+1,\downarrow} - c_{x,y,\downarrow} c_{x,y+1,\uparrow}) \right\}, \quad (15)$$

with  $t' < 0$  giving the analogous singlet extended- $s$  operator. With different relative phases, one can also obtain  $m = 0$  triplet pairs; because quantum spin fluctuations are not included in the  $t - J_z$  model, the two cases cannot be differentiated at this level.

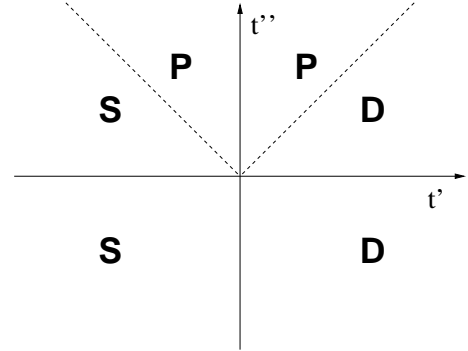


FIG. 1. Hole pair symmetry in the strong-coupling limit of the  $t' - t'' - J_z$  model as a function of  $t'$  and  $t''$ . Here, “D” denotes  $d_{x^2-y^2}$ , “P” denotes  $p_x$  or  $p_y$ , and “S” denotes extended- $s$ .

For the more general  $t' - t'' - J_z$  model, one obtains the (unnormalized) wave functions

$$|\psi_{k_x,k_y}^\pm\rangle = e^{-\frac{\pi i k_x x}{L}} (4t') s_x s_y |h_{k_x,k_y}\rangle + e^{-\frac{\pi i k_y y}{L}} \left[ (2t'')(s_y^2 - s_x^2) \pm \tau_{x,y} \right] |v_{k_x,k_y}\rangle \quad (16)$$

with energies

$$\epsilon_{k_x,k_y}^\pm = (-2t'')(1 - s_x^2 - s_y^2) \pm \tau_{x,y}, \quad (17)$$

where  $s_x = \sin(\pi k_x/L)$ ,  $s_y = \sin(\pi k_y/L)$ , and

$$\tau_{x,y} = 2 \left\{ (t'')^2 (s_x^2 - s_y^2)^2 + 4(t')^2 s_x^2 s_y^2 \right\}^{\frac{1}{2}}. \quad (18)$$

As a function of  $t'$  and  $t''$ , we find that the ground state symmetry of the pair is as shown in Fig. 1. The  $p$ -wave pair operators can be either  $p_x$

$$\frac{1}{L} \sum_{x,y} e^{-\frac{2\pi i k_y y}{L}} a_{x,y} (a_{x+1,y} - a_{x-1,y}) \quad (19)$$

or  $p_y$

$$\frac{1}{L} \sum_{x,y} e^{-\frac{2\pi i k_x x}{L}} a_{x,y} (a_{x,y+1} - a_{x,y-1}). \quad (20)$$

The  $p_x$  states have energies independent of  $k_y$ , and the  $p_y$  states have energies independent of  $k_x$ . Both  $p$ -wave pair operators change sign under a 180 degree rotation.

We next consider the strong-coupling limit of the  $t - J_z$  model. To lowest order, we find that this maps onto the above strong-coupling limit of the  $t' - t'' - J_z$  model with

$$t'_{eff.} = t''_{eff.} = \frac{2}{3} \left( \frac{t^2}{J_z} \right). \quad (21)$$

From Eq. 17, the lower band of the pair excitation spectrum then becomes flat, with wave functions

$$|\psi_{k_x, k_y}^- \rangle = \frac{1}{\sqrt{2}} \left\{ e^{-\frac{\pi i k_x x}{L}} s_y |h_{k_x, k_y} \rangle - e^{-\frac{\pi i k_y y}{L}} s_x |v_{k_x, k_y} \rangle \right\}. \quad (22)$$

Flat bands were also found [17,18] for related models and/or treatments. In [15], a five-fold degeneracy of strong-coupling  $t - J_z$  pairs of  $d$  or  $p$  symmetry was noted.

We see from Eq. 21 that, to lowest order, the strong-coupling  $t - J_z$  model lies on the (rightmost) boundary in Fig. 1 between  $d$ -wave and  $p$ -wave symmetry. In the next higher order, neglecting constant additive terms, the energies of the lower band separate into

$$\epsilon_{k_x, k_y}^- = \left( -\frac{8}{45} \right) \left( \frac{t^4}{J_z^3} \right) (2 - c_x - c_y)^{-1} \{ c_x^2 + c_y^2 + 4c_x c_y - 31c_x - 31c_y + 56 \}, \quad (23)$$

where here  $c_x = \cos(2\pi k_x/L)$  and  $c_y = \cos(2\pi k_y/L)$ . We then find (in agreement with [15]) that the pure  $d$ -wave ( $t' > 0$ ) state of Eq. 14 is selected as the ground state. However, the closeness to  $p$ -wave symmetry may provide an explanation for the low-energy  $p$ -wave “quasi-pair” peaks seen numerically in small  $t - J$  and  $t - J_z$  clusters [13]. Because of this similar  $t - J$  and  $t - J_z$  behavior, referring to Fig. 1 and assuming ground state pairs of pure symmetry, we predict that adding the appropriate  $t'$  and/or  $t''$  to the  $t - J_z$  or  $t - J$  models with  $J_z/t$  or  $J/t$  sufficiently large should drive the models to  $p$ -wave hole pair symmetry, and perhaps even  $p$ -wave superconductivity. (In one dimension, a n.n.n.  $t' > 0$  will also give  $p$ -wave hole-pair symmetry in the  $J_z \gg |t|, |t'|$  limit.)

One can perturbatively construct increasingly extended quasi-pair states for the  $t - J_z$  model. Combining results for the n.n.  $d$ -wave pair operators for ground states  $|\Phi_a \rangle$  and  $|\Phi_b \rangle$ , one finds the lowest order correction for the singlet pair operator of Eq. 15

$$\begin{aligned} & \left( -\frac{4}{3} \right) \left( \frac{t}{J_z} \right) \left( \frac{1}{L} \right) \sum_{x,y,\sigma} \sigma \\ & \left\{ (c_{x+1,y,\sigma}^\dagger c_{x+1,y,-\sigma} - c_{x,y+1,-\sigma}^\dagger c_{x,y+1,\sigma}) \right. \\ & \quad c_{x+1,y+1,\sigma} c_{x,y,\sigma} \\ & \quad \left. + (c_{x+1,y,\sigma}^\dagger c_{x+1,y,-\sigma} - c_{x,y-1,-\sigma}^\dagger c_{x,y-1,\sigma}) \right. \\ & \quad \left. c_{x+1,y-1,\sigma} c_{x,y,\sigma} \right\}. \end{aligned} \quad (24)$$

When operating on the appropriate Néel state, each of the above terms consists of a diagonal hole pair “dressed” with a singlet pair of electrons straddling the bond connecting the pair of holes, as was recently found in numerical  $t - J$  simulations [8]. We note that the contribution from pairs a distance of two lattice sites apart, nominally also of order  $t/J_z$ , vanishes identically in this order. This may provide an explanation for why only n.n. and diagonal hole correlations appear to dominate in the  $t - J$  model near half filling for moderate to large  $J/t$  [8,19].

If one adds the necessary terms to the operator of Eq. 24 to impose rotational invariance, one obtains the composite pair operator invented in [19] to give a diagonal singlet pair with  $d_{x^2-y^2}$  symmetry. The non-invariant operator of Eq. 24, which emerges naturally from perturbation theory, also has  $d_{x^2-y^2}$  symmetry.

We also note that, since we calculate energy spectra and wave functions, our results and approach can be used to calculate finite-temperature and real frequency properties. However, we do not pursue that here.

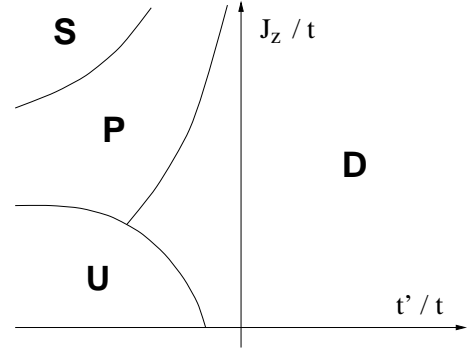


FIG. 2. Qualitative diagram of predicted hole pair symmetry for the  $t - t' - J_z$  model. “D”, “P”, and “S” denote the same as in Fig. 1, and no prediction is made for region “U”.

As one step towards investigating the range of validity of our approach, we performed analytic calculations of the  $t - t' - J_z - J_\perp$  model (see Eq. 6) on a 2x2 plaquette. In general, we found that ground states remained smoothly connected as  $J_z$  was reduced from strong coupling and also as  $J_\perp$  was turned on.  $t - J$  numerical results [15,19] also indicate that features of the strong-coupling limit may persist down to intermediate coupling ( $J/t \approx 0.4-0.5$ ). Together, the above support the strong-coupling  $t - t' - t'' - J_z$  model as a useful starting point for exploring the intermediate-coupling  $t - t' - t'' - J$  model. Based on this and our strong-coupling results

(and, again, assuming pairs of pure symmetry), we show in Fig. 2 qualitative predictions of the hole pair symmetry for the  $t - t' - J_z$  model. We believe these predictions apply to the  $t - t' - J$  model as well, with a comparatively smaller  $p$ -wave region due to larger energy differences between  $t - J$   $p$ -wave and  $d$ -wave pair states [13]. An additional  $t'' > 0$  would enlarge the  $p$ -wave region.

Reductions from CuO<sub>2</sub> three-band models [20], as well as comparison with ARPES results for a single doped hole [21], suggest that  $|t'/t|$  and  $|t''/t|$  may be substantial.  $t > 0$ , and estimates for  $t'$  and  $t''$  are typically in the ranges  $t' \approx (-0.1)t - (-0.5)t$ , and  $t'' \approx 0.0 - (0.3)t$ . Both these signs of  $t'$  and  $t''$  could tend to drive the pairing symmetry to  $p$ -wave, raising the issue of the hole pair symmetry in the intermediate-coupling regime. ( $s$ -wave is also possible, though we believe it less likely at intermediate coupling.) It would be interesting to numerically explore whether the symmetry of two doped holes in the  $t - t' - t'' - J$  model is in fact  $d$ -wave for the experimentally relevant values of  $t, t', t''$ , and  $J$  (e.g.,  $J/t \approx 0.4$ ). Drawing conclusions from exact diagonalization may be challenging due to finite-size effects: either  $s$ -wave or  $p$ -wave hole pair symmetries were found on lattices of sizes 16, 18, and 20 for the  $t - t' - J$  model with realistic parameters [22]. Another possible tool is higher order numerical ground state perturbation theory [15]. If the symmetry were established to be  $p$ -wave rather than  $d$ -wave, it would suggest that the  $t - t' - t'' - J$  model by itself could be incomplete as a model for high- $T_c$  superconductivity. In that case, one possibility for restoring  $d$ -wave symmetry could be the addition of electron-phonon coupling in the  $d$ -channel [23]. In either case, it may also be of interest to explore whether the existence of or nearness to  $p$ -wave symmetry, which effectively reduces the dimensionality of the hole pair wave function from 2D to 1D, might play a role in the “striping” recently observed in certain of the high- $T_c$  cuprates [24].

In summary, we have investigated analytically the pair symmetry and excitation spectra of two holes doped into the half-filled  $t - t' - t'' - J_z$  model in the strong-coupling limit. In lowest order, this reduces to considering the  $t' - t'' - J_z$  model, where we found regions of  $d$ -wave,  $s$ -wave, and  $p$ -wave symmetry. We next found that the  $t - J_z$  model in lowest order was on the boundary between  $d$ -wave and  $p$ -wave pair symmetry, with a flat lower pair excitation spectrum. In higher order,  $d$ -wave pairing was selected. However, because of the closeness to  $p$ -wave symmetry, we predict that the appropriate  $t'$  and/or  $t''$  added to the  $t - J_z$  or  $t - J$  models with intermediate to large  $J_z$  or  $J$  should drive them into  $p$ -wave pairing, and perhaps even  $p$ -wave superconductivity. We constructed a perturbative correction to the nearest neighbor  $d$ -wave pair, and compared with the  $d$ -wave composite operator invented in [19]. We explored ranges of validity of this perturbative approach using a 2x2 plaquette and results from other work [15,19]. Lastly, we discussed implications for the experimentally relevant parameter regime. These included the possibility of  $p$ -wave symme-

try for two doped holes, which would suggest that the  $t - t' - t'' - J$  model could be incomplete as a high- $T_c$  model, and the possible relevance of our results to “striping”.

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